CONF-810628--2

LA-UR-81-1409

MASTER

TITLE: k-LINE ITERATIVE METHODS: A CONJUGATE-GRADIENT APPROACH

AUTHOR(S): David Kratzer, Seymour V. Parter, and Michael Steuerwalt

SUBMITTED TO: 4th IMACS International Symposium on Computer Methods for Partial Differential Equations

Bethlehem, Pennsylvania
June 30 - July 2, 1981

March 29, 1981

University of California

LOS ALAMOS SCIENTIFIC LABORATORY
Post Office Box 1663 Los Alamos, New Mexico 87545
An Affirmative Action/Equal Opportunity Employer

Form No. 836 R3
St. No. 2629

UNITED STATES
DEPARTMENT OF ENERGY

k-LINE ITERATIVE METHODS: A CONJUGATE-GRADIENT APPROACH(*)

David Kratzer
Department of Mathematics, Hardin College, Searcy, AR 72143
Seymour V. Parter
Department of Mathematics, University of Wisconsin, Madison, WI 53706
Michael Steuerwalt
University of California
Los Alamos National Laboratory, MS 608, Los Alamos, NM 87545

Abstract

We study the generalized conjugate gradient scheme based on the k-line block Jacobi splitting $A = M-N$ for solving model two-dimensional parabolic and elliptic difference equations $AU = \vec{F}$. A represents the matrix $ch^{\alpha}-h^2\Delta_h$. Eigenvalues of $M^{-1}N$ cluster, and the cluster radii decrease as ch^{α} or k increases. We discuss computations with $k = 4, 8, 16, 32$, and $ch^{\alpha} = 0, h, 2$.

(*) This work was supported by the U.S. Department of Energy under Contract W-7405-Eng-36, and by the Office of Naval Research under Contract N00014-76-C-0341.

1. Introduction

Direct iterative methods for solving the system

$$AU = \vec{F} \tag{1.1}$$

split the matrix A into a difference

$$A = M - N. \tag{1.2}$$

Convergence of the methods is governed by the eigenvalues of the matrix $M^{-1}N$. While studying block iterative methods for two-dimensional elliptic and parabolic problems, Parter and Steuerwalt[10] noticed that when the model problem has a form of strong diagonal dominance, eigenvalues of the k-line block Jacobi matrix form clusters. The generalized conjugate gradient method[2] based on this splitting therefore should be an effective way to solve the difference equations, for it is well known that clustering improves convergence of the conjugate gradient iterates. Here we present some numerical experiments, together with estimates of the eigenvalues, that not only confirm this expectation but also show that some clusters themselves coalesce.

The model problem

Impose a mesh with uniform spacing

$$h := 1/(P + 1) \tag{1.3}$$

on the unit square $\bar{\Omega} := \{(x,y) \in \mathbb{R}^2 : 0 \le x, y \le 1\}$, and let $(x_i,y_j) := (ih,jh)$. The interior mesh points Ω_h and the discrete boundary $\partial\Omega_h$ are the sets $\Omega_h := \{(x_i,y_j) : 1 \le i, j \le P\}$ and $\partial\Omega_h := \{(x_i,y_j) : i = 0$ or $= P+1$, or $j = 0$ or $= P+1\}$. A mesh vector $U = (U_{i,j})$ is a function defined on the entire mesh $\bar{\Omega}_h := \Omega_h \cup \partial\Omega_h$.

The discrete Laplace operator is defined at points in Ω_h by

$$[\Delta_h U]_{i,j} := (U_{i-1,j} - 2U_{i,j} + U_{i+1,j})/h^2 + (U_{i,j-1} - 2U_{i,j} + U_{i,j+1})/h^2.$$

We suppose that $c \ge 0$ and $0 \le \alpha \le 2$ are given constants and we define an elliptic difference operator L_h by

$$[L_h U]_{i,j} := ch^{\alpha-2}U_{i,j} - [\Delta_h U]_{i,j}. \tag{1.4}$$

Note that, although the mesh vector U is defined on $\bar{\Omega}_h$, the vectors $\Delta_h U$ and $L_h U$ are defined only at the interior mesh points. Given a mesh vector F, the model problem is to find a mesh vector U satisfying

$$L_h U = F \text{ in } \Omega_h, \quad U = 0 \text{ on } \partial\Omega_h. \tag{1.5}$$

After choosing an ordering of the mesh points, we let A be the matrix representing h^2L_h, and get a system (1.1) of order P^2. $\vec{F}$ indicates the result of ordering the components of h^2F. Using a standard ordering, A can be written as the P×P block tridiagonal matrix

$$A = [-E, T, -E]_P \tag{1.6}$$

whose entries are matrices of order P: T is the P×P tridiagonal matrix $T := [-1, 4+ch^{\alpha}, -1]_P$ and E denotes the P×P identity matrix.

The significance of α

If $\alpha = 2$, L_h given by (1.4) is a regular elliptic difference operator. Some evaluation of different splittings has been attempted for regular problems when A is symmetric and positive definite.[4,8] Our estimates show that the k-line Jacobi splitting works well for the model operator (1.4).

If $\alpha < 2$, then L_h is a singularly perturbed operator, A is strongly diagonally dominant, and the eigenvalues of $M^{-1}N$ bunch tightly. The case $\alpha = 0$ arises in applying block iterative methods to elliptic problems in higher dimensions.[10] Discrete-time schemes for the parabolic operator $c_0\partial/\partial t-\Delta$ may give at each time level an elliptic operator $c/\tau-\Delta$. Conditions on the ratio h^2/τ then lead to singularly perturbed operators (1.4) with $0 < \alpha < 2$. For example, a common choice of τ in the Crank-Nicolson method yields $\alpha = 1$.

When $0 < \alpha \leq 2$, the spectral radius ρ of $M^{-1}N$ for the k-line Jacobi scheme is[11] $\rho = 1-kh^{\alpha}\text{const}$. Consequently $O(1/(kh^{\alpha})^{1/2})$ steps of the related successive overrelaxation method with best ω are needed to reduce any initial error by a fixed factor. In contrast, if $M^{-1}N$ has $2/h$ distinct eigenvalues, then in principle the conjugate gradient method converges to the solution from any initial guess in at most $2/h$ steps. One hopes for similar behavior, though not finite termination in so few steps, if the eigenvalues form $2/h$ clusters.

In section 2 we discuss some numerical experiments that suggest the eigenvalues of $M^{-1}N$ for the k-line Jacobi splitting cluster strongly. A description of this splitting for the model problem, a statement of the generalized conjugate gradient method and the optimality theorem, and an appraisal of the effect of clustering appear in section 3. We sketch in section 4 a derivation of bounds on the size and number of clusters.

Our method of analysis seems limited to the model problem. Nevertheless, we expect that the clustering results we outline here hold more generally.

2. Numerical experiments

We used the generalized conjugate gradient algorithm and the k-line Jacobi splitting (3.3) to solve the equation (1.1) that comes from the model problem (1.5) on a mesh with $P = 128$. We chose for ch^{α} the values 0, h, and 2. These typical values correspond, respectively, to a regular elliptic problem, a singularly perturbed elliptic problem arising from a discrete-time scheme for a parabolic problem, and a singularly perturbed elliptic problem that comes from treating the model three-dimensional operator by a block iterative method whose basic block is a plane.

To minimize the effects of roundoff, we set $\tilde{F} = 0$; hence the solution is $U = 0$, and the error of each iterate $U^{(\nu)}$ is the iterate itself. We took $U^{(0)}$ to be the vector with components all 1. Computations with different $\tilde{F}$ or $U^{(0)}$ showed very similar behavior. The calculations were done on the Cray-1 at Los Alamos.

In each figure the horizontal axis is the number ν of iterations, and the vertical axis is the log of the Euclidean norm or A-norm (see (3.6)) of the error $E^{(\nu)} := U-U^{(\nu)}$, or the Euclidean norm of the residual $R^{(\nu)} := \tilde{F}-AU^{(\nu)}$, for various values of k and of ch^{α}.

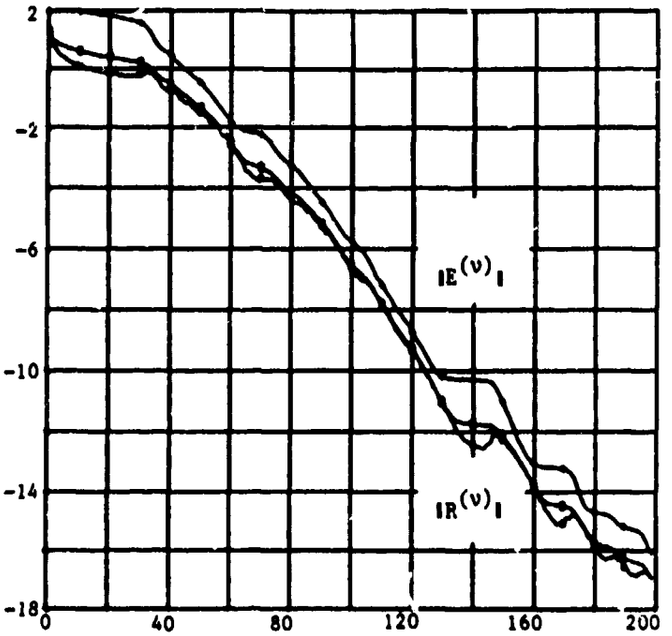

Figure 1. $\|E^{(\nu)}\|$, $\|E^{(\nu)}\|_A$, and $\|R^{(\nu)}\|$ ($ch^{\alpha} = 0$, $k = 4$)

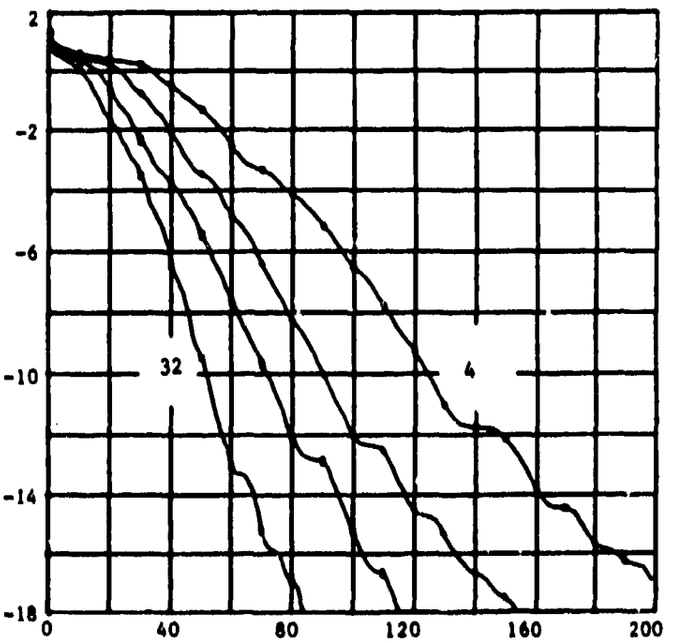

Figure 2. $\|E^{(\nu)}\|_A$ for various k ($ch^{\alpha} = 0$)

The relation between $\|E^{(\nu)}\|_A$, $\|E^{(\nu)}\|$, and $\|R^{(\nu)}\|$ is shown in Figure 1. Note that $\|E^{(\nu)}\|_A$ is monotone; this is predicted by the Optimality Theorem 3.2.[2,5,6]

In contrast, the residuals bounce around and even increase just before the "cliffs." One has access only to the residuals in practice, and should be careful not to terminate the algorithm just before a dramatic improvement in the error is obtained.

Figure 2 displays $\|E^{(\nu)}\|_A$, and Figure 3 plots $\|R^{(\nu)}\|$, for $ch^{\alpha} = 0$ and different k. Only $\|R^{(\nu)}\|$ is plotted in the remaining graphs.

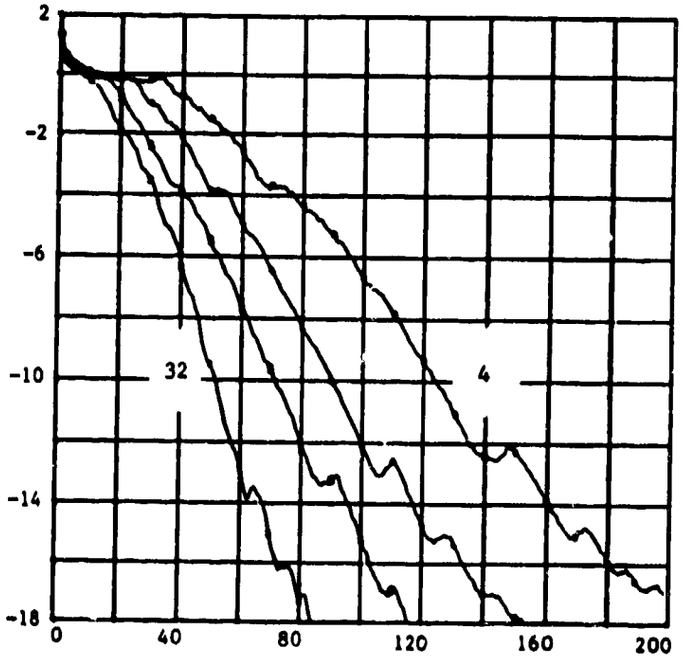

Figure 3. $\|R^{(\nu)}\|$ for various k ($ch^{\alpha} = 0$)

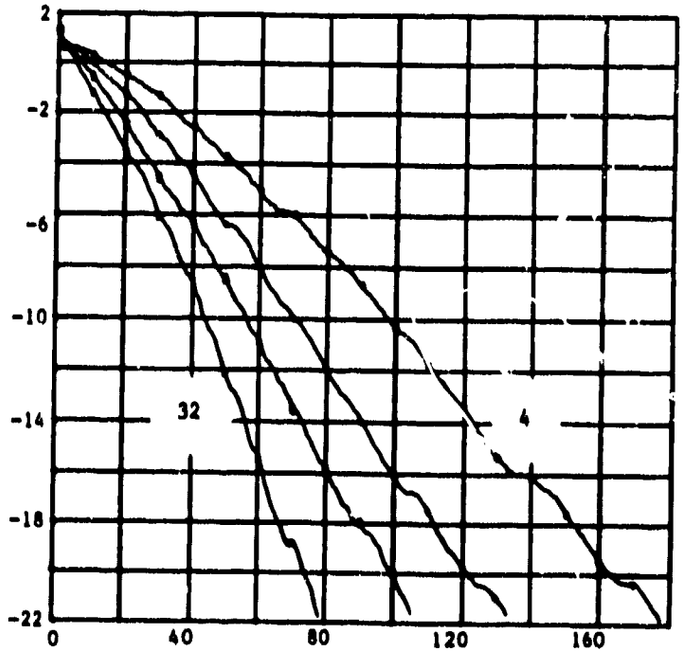

Figure 4. $\|R^{(\nu)}\|$ for various k ($ch^{\alpha} = h$)

Figures 3-5 show the effect of increasing k, for fixed ch^{α}, while Figures 6-7 display the result of increasing ch^{α} for fixed k.

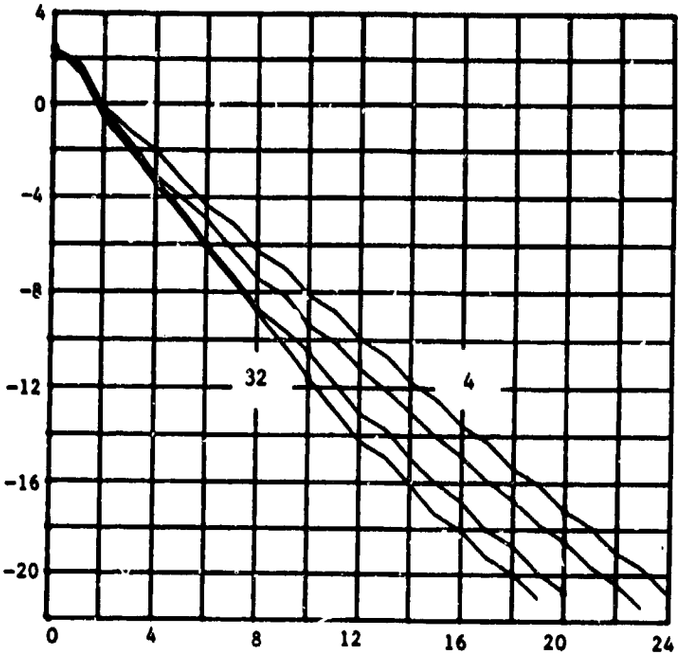

Figure 5. $\|R^{(\nu)}\|$ for various k ($ch^{\alpha} = 2$)

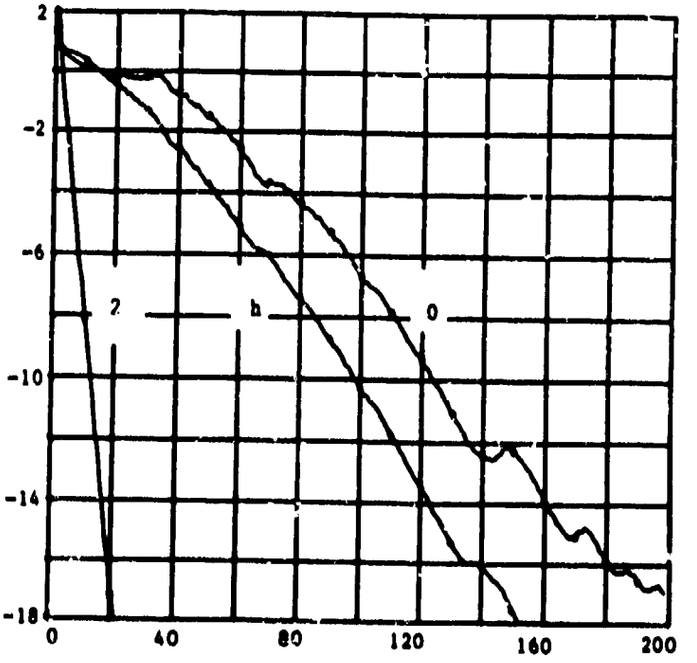

Figure 6. $\|R^{(\nu)}\|$ for various ch^{α} (k = 4)

The "cliffs and plateaus" of these graphs have been noticed before.[3,5,8] Their location with respect to the number of iterations closely reflects the number n of distinct clusters of eigenvalues of $M^{-1}N$. The

analysis of section 4 demonstrates for the k-line block Jacobi splitting that eigenvalues will cluster, and indicates that cliffs should appear every n steps, where n is at worst 2P+1. When n is much less than 2P, we suspect that the clusters themselves are coalescing.

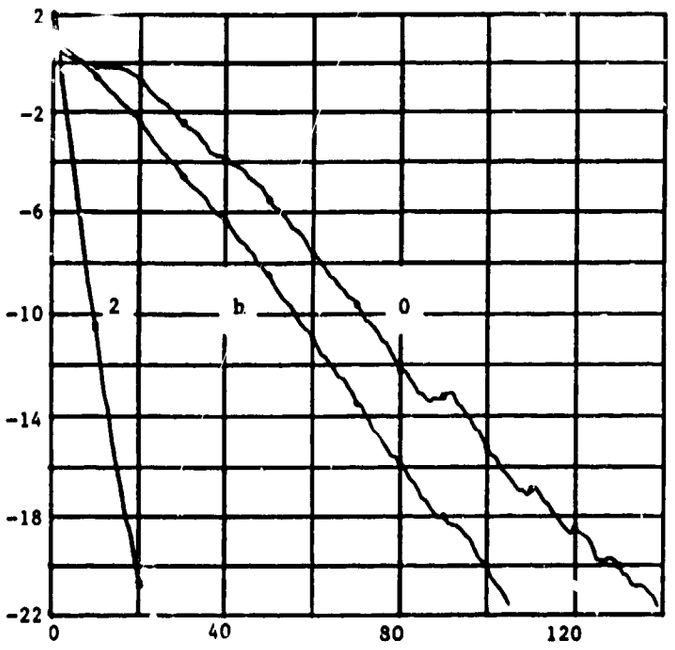

Figure 7. $|R^{(\nu)}|$ for various ch^{α} (k = 16)

The plots show that convergence improves as ch^{α} or k increases; they also suggest that n is significantly less than 2P. When ch^{α} is 0 or h, it appears that n ≅ 75, 55, 45, 35 for k = 4, 8, 16, 32, respectively. Convergence is so rapid that no plateau appears when ch^{α} = 2. It is possible that in fact n is about twice as big as we now believe; to check this point, computations in high precision are being done. But even if n ≅ 150, about 40% of the clusters have coalesced.

3. The conjugate gradient method with k-line blocks

The k-line block Jacobi splitting

In the horizontal k-line block structure[9,10,11] each block of U comprises the unknowns $U_{i,j}$ associated with the points (x_i, y_j) on k consecutive horizontal grid lines. Let k be a divisor of P, so that

$$P = kQ \text{ for some integer } Q. \tag{3.1}$$

The k-line blocks are $\tilde{U}_s := \{U_{i,k(s-1)+j} : 1 \le i \le P, 1 \le j \le k\}$ $(1 \le s \le Q)$. This decomposition of U induces a block structure in A. If E is the P×P identity and S and R are the k×k block matrices

$$S := [-E, T, -E]_k, \quad R := \begin{vmatrix} 0 & E \\ 0 & 0 \end{vmatrix},$$

then A is the block tridiagonal matrix $[-R, S, -R^t]_Q$ whose entries are matrices of order kP.

A direct iterative scheme for solving (1.1) splits A as in (1.2). Choosing a first guess $U^{(0)}$, we get a sequence $\{U^{(\nu)}\}$ by solving $MU^{(\nu+1)} = NU^{(\nu)}+\tilde{F}$. When A is nonsingular the sequence converges to the solution of (1.1) independently of $U^{(0)}$ if and only if

$$\rho := \max \{|\lambda| : \det(\lambda M - N) = 0\},$$

the spectral radius of $M^{-1}N$, satisfies $\rho < 1$. Hence we are led to study the eigenvalue problem

$$\lambda MU = NU. \tag{3.2}$$

In the k-line Jacobi scheme, A splits into the block matrices

$$M := [0, S, 0]_Q, \quad N := [R, 0, R^t]_Q; \tag{3.3}$$

it is evident from (1.6) and (3.3) that A and M are symmetric and positive definite and N is nonnegative. Hence $\rho < 1$, and we may rewrite (3.2) to get

$$\sigma AU = NU, \quad \sigma := \lambda/(1 - \lambda). \tag{3.4}$$

Furthermore, nonzero eigenvalues of $M^{-1}N$ occur in signed pairs $\pm\lambda$.[1,9,11,12,13]

The generalized conjugate gradient method

Splittings (1.2) also play a role in the generalized conjugate gradient scheme.[2] The method assumes A to be symmetric positive definite. In this section M is any symmetric positive definite matrix of the same order ℓ as A.

Algorithm 3.1. The generalized conjugate gradient method. Choose M. Let $U^{(0)}$ be a first guess at the solution U of (1.1), set $\nu := 0$, and fix an arbitrary $V^{(-1)}$. Generate the sequence $\{U^{(\nu)}\}$ by the following steps. Step 1: Obtain $Z^{(\nu)}$ as the solution of

$$MZ^{(\nu)} = \tilde{F} - AU^{(\nu)}; \tag{3.5}$$

stop if $Z^{(\nu)} = 0$. Step 2: Compute

$$\beta_\nu := \begin{cases} 0 & \text{if } \nu = 0 \\ (Z^{(\nu)}, MZ^{(\nu)})/(Z^{(\nu-1)}, MZ^{(\nu-1)}) & \text{if } \nu > 0, \end{cases}$$

$$V^{(\nu)} := Z^{(\nu)} + \beta_\nu V^{(\nu-1)}.$$

Step 3: Compute

$$\alpha_\nu := (Z^{(\nu)}, MZ^{(\nu)})/(V^{(\nu)}, AV^{(\nu)}),$$
$$U^{(\nu+1)} := U^{(\nu)} + \alpha_\nu V^{(\nu)},$$

advance ν, and return to step 1. □

Note that $MZ^{(\nu)} = 0$ iff $U^{(\nu)}$ solves (1.1). The coefficients α_ν and β_ν are chosen so that $(Z^{(i)}, MZ^{(j)}) = 0$ if $i \neq j$. It follows from this M-orthogonality property that $\{U^{(\nu)}\}$ converges to the solution U of (1.1) in at most ℓ steps. In practice, roundoff causes a gradual loss of M-orthogonality and consequent failure of the finite termination property; hence we view the method as an iterative scheme.[2,3,5]

The key result about this scheme is the Optimality Theorem, which -- neglecting roundoff -- describes the convergence of $\{U^{(\nu)}\}$. We let $\mathcal{P}_\nu$ be the set of real polynomials of degree no greater than ν, and recall that any positive definite matrix B defines a norm by

$$\|X\|_B := (X, BX)^{1/2}. \tag{3.6}$$

Theorem 3.2. The optimality theorem.[2,5,6] Denote by U the solution of (1.1), and by $\{U^{(\nu)}\}$ the generalized conjugate gradient iterates. Then

$$\|U^{(\nu+1)} - U\|_A^2 \tag{3.7}$$
$$= \min \{\|[I - Kp(K)](U^{(0)} - U)\|_A^2 : p \in \mathcal{P}_\nu\},$$

where

$$K := M^{-1}A = I - M^{-1}N. \quad \square \tag{3.8}$$

Let $m(\kappa)$ be the minimal polynomial of K, so that $m(K) = 0$. Let $\kappa_1, \ldots, \kappa_n$ be the distinct eigenvalues of K. Because K is similar to a real symmetric matrix (hence diagonalizable), $m(\kappa) = \Pi_{j=1}^{n}(\kappa - \kappa_j)$. No κ_j is zero, so $m(\kappa) = [1 - \kappa p(\kappa)]\Pi_j(-\kappa_j)$ for some particular $p \in \mathcal{P}_{n-1}$. These remarks prove:

Corollary 3.3. If K has exactly n distinct eigenvalues, then $U^{(n)} = U$ and so the generalized conjugate gradient method converges in at most n steps. □

The effect of clustering

The original conjugate gradient method[6] set $M = I$. Corollary 3.3 says to pick M so that K has as few distinct eigenvalues as possible, subject to the condition that (3.5) be "easy" to solve. Hence the choice $M = A$ is not practical. But if the eigenvalues of K cluster about n distinct values $\{\hat{\kappa}_j\}$, $\|U^{(n)} - U\|_A$ should be small. Now we quantify this expectation.

By (3.8) the eigenvalues λ_i of $M^{-1}N$ and κ_i of K are related according to the equation $\kappa = 1 - \lambda$. We therefore impose conditions on the eigenvalues of K in terms of λ_i. These conditions are motivated by the facts regarding the k-line Jacobi splitting (3.3) set down before. We assume that the spectral radius ρ of $M^{-1}N$ is less than 1, the nonzero eigenvalues of $M^{-1}N$ occur in signed pairs $\pm\lambda_j$, and all the eigenvalues of $M^{-1}N$ cluster. Precisely, we suppose there are nonnegative numbers δ_r and $\hat{\lambda}_r$, $1 \leq r \leq s$, so that for any nonzero λ_i there is an r for which

$$|\lambda_i - \hat{\lambda}_r| \leq \delta_r \quad \text{or} \quad |\lambda_i + \hat{\lambda}_r| \leq \delta_r. \tag{3.9}$$

Without loss of generality we may take each $\hat{\lambda}_r < 1$. To determine the behavior of $\{U^{(\nu)}\}$, we appraise the right hand side of (3.7). Clearly

$$\hat{m}(\kappa) := (1 - \kappa) \Pi_{j=1}^{s} \frac{(\kappa - [1+\hat{\lambda}_j])(\kappa - [1-\hat{\lambda}_j])}{(1 - \hat{\lambda}_j^2)}$$

has the required form $1 - \kappa p(\kappa)$. Fix any eigenvalue κ_i of K. Evidently $\kappa_i = 1$ iff $\lambda_i = 0$, and then $\hat{m}(\kappa_i) = 0$. If $\kappa_i \neq 1$, then $\lambda_i \neq 0$, and by (3.9) for some r

$$|\hat{m}(\kappa_i)| \leq \frac{|\lambda_i||\lambda_i - \hat{\lambda}_r||\lambda_i + \hat{\lambda}_r|}{1 - \hat{\lambda}_r^2} Q(\lambda_i, r)$$
$$\leq 2\delta_r Q(\lambda_i, r)/(1 - \hat{\lambda}_r^2),$$

where

$$Q(\lambda, r) := \Pi_{j \neq r} \frac{|\lambda_i^2 - \hat{\lambda}_j^2|}{1 - \hat{\lambda}_j^2}. \tag{3.10}$$

It follows that in some norm (e.g., the Euclidean norm of the diagonal matrix to which K is similar) $\hat{m}(K)$ is of order $\max_r\{\delta_r\}$ in magnitude, and therefore small if the clusters are small. By the Optimality Theorem 3.2, then, $\|U^{(2s+1)} - U\|_A^2 = O(\max\{\delta_r : 1 \leq r \leq s\})$.

Thus we need to determine whether the eigenvalues of K, or equivalently the eigenvalues of $M^{-1}N$, cluster for the k-line block Jacobi splitting (3.3).

4. Estimates of the eigenvalues

Because the spectral radius of $M^{-1}N$ is less than 1, we can convert the eigenvalue problem (3.2) for λ into the eigenvalue problem (3.4) for σ. We restrict

attention to the case $k \geq 3$. The test vectors $U^{(r)}_{i,j} := \psi^{(r)}_j \sin \pi i r h$ show that each σ is an eigenvalue of

$$\sigma B[\beta(r)]\psi^{(r)} = \tilde{N}\psi^{(r)} \tag{4.1}$$

for some r, $1 \leq r \leq P$. Here $\psi^{(r)} \in \mathring{R}^P$ and

$$\beta(r) := 2(2 - \cos \pi r h) + ch^{\alpha}; \tag{4.2}$$

$B[\beta]$ is the tridiagonal matrix $[-1, \beta, -1]$ of order P. $\tilde{N}$ is also a tridiagonal matrix of order P, whose action on vectors $\phi := (\phi_1, \phi_2, \ldots, \phi_P)^t$ is given by

$$[\tilde{N}\phi]_{ks+\sigma} := \begin{cases} \phi_{ks+1} & 1 \leq s \leq Q-1,\ \sigma = 0 \\ \phi_{ks} & 1 \leq s \leq Q-1,\ \sigma = 1, \end{cases}$$

$$[\tilde{N}\phi]_j := 0 \quad \text{for any other subscript } j.$$

B is positive definite and $\tilde{N}$ is symmetric, so for each r there are P linearly independent eigenvectors ψ and P (counting multiplicities) associated eigenvalues σ of (4.1). It follows that this separation of variables procedure provides all the eigenvectors of (3.4).

Before proceeding, we recall some properties of the Gaussian algorithm for tridiagonal systems.[7,12]

Lemma 4.1. Let $k \geq 3$. Consider the linear system

$$-\phi_{j-1} + \beta\phi_j - \phi_{j+1} = 0 \quad (1 \leq j \leq k-2),$$

where $\beta \geq 2$, ϕ_0, and ϕ_{k-1} are given. Define $\{E_j\}$ by

$$E_0 := 0, \quad E_j := 1/(\beta - E_{j-1}) \quad (1 \leq j \leq k-2) \tag{4.3}$$

and set

$$a_k := E_1 E_2 \cdots E_{k-2}, \quad b_k := E_{k-2}. \tag{4.4}$$

Then

$$\phi_1 = a_k\phi_{k-1} + b_k\phi_0, \quad \phi_{k-2} = b_k\phi_{k-1} + a_k\phi_0.$$

Furthermore, $\{E_j\}$ is a monotone increasing sequence in the interval $[0,1]$, and as $k \to \infty$

$$b_k \uparrow b_\infty := (\beta - (\beta^2 - 4)^{1/2})/2, \quad a_k \downarrow 0.$$

When $\beta > 2$, this convergence is exponentially fast, and when $\beta = 2$ we have $a_k = 1/(k-1)$, $b_k = (k-2)/(k-1)$. □

Now fix r and define β by (4.2). We use Lemma 4.1 to eliminate those equations and corresponding unknowns in (4.1) for which the right hand side is zero.

Lemma 4.2. Let $\sigma \neq 0$ be an eigenvalue and ψ the associated eigenvector of (4.1), and set

$$\gamma := 1 + 1/\sigma, \tag{4.5}$$

$$\xi_{2s-1} := \psi_{ks}, \quad \xi_{2s} := \psi_{ks+1} \quad (1 \leq s \leq Q-1).$$

Then ξ must satisfy the homogeneous system $\tilde{A}\xi = 0$, where $\tilde{A} := \tilde{A}(\beta,\gamma)$ is the block tridiagonal matrix

$$\tilde{A} := [C, D_i, C^t] \quad (1 \leq i \leq Q-1)$$

with 2×2 blocks

$$D_1 := \begin{vmatrix} \beta - b_{k+1} & -\gamma \\ -\gamma & \beta - b_k \end{vmatrix}, \quad D_i := \begin{vmatrix} \beta - b_k & -\gamma \\ -\gamma & \beta - b_k \end{vmatrix},$$

$$D_{Q-1} := \begin{vmatrix} \beta - b_k & -\gamma \\ -\gamma & \beta - b_{k+1} \end{vmatrix}, \quad C := \begin{vmatrix} 0 & -a_k \\ 0 & 0 \end{vmatrix}. \ \square$$

Nonzero eigenvalues σ of (4.1) thus correspond to values of γ for which $\tilde{A}$ is singular. We bound γ by a Gerschgorin argument, and so estimate nonzero eigenvalues λ of (3.2) -- for $\gamma = 1/\lambda$ from (4.5) and (3.4).

Theorem 4.3. If the matrix $\tilde{A}$ is singular, then any nonzero eigenvalue λ of $M^{-1}N$ satisfies

$$||\lambda| - \hat{\lambda}_r| \leq \delta(\beta,k)/(\beta(r) - b_\infty) \leq \delta(\beta,k), \tag{4.6}$$

where

$$\delta(\beta,k) := a_k + (b_\infty - b_{k+1}), \tag{4.7}$$

$$\hat{\lambda}_r := 2/[\beta(r) + (\beta(r)^2 - 4)^{1/2}]. \ \square$$

We see then that nonzero eigenvalues λ of (3.2) cluster about the 2P values $\pm\hat{\lambda}_r$, $1 \leq r \leq P$. The situation described after Corollary 3.3 now holds, and the numbers δ_r of that discussion are the values $\delta(\beta(r),k)$ defined by (4.7), (4.3), and (4.4) with $\beta = \beta(r)$. So even in the worst case, in which $c = 0$ and $\min_r\{\beta(r)\} = 4 - 2\cos \pi h \cong 2 + (\pi h)^2$, we have no more than 2s+1 clusters with $s = P$ and $\delta_r = O(h)$.

In fact, the eigenvalues bunch in another way as well. $\hat{\lambda}_r$ is a continuous function of rh, and $|\hat{\lambda}_r - \hat{\lambda}_q| = O(h^2)$ when r and q are near P. So the clusters themselves coalesce, for their centers have only $O(h^2)$ separation for large r. The plots in section 2 indicate that many of the clusters coalesce. In Figure 8 r is the horizontal and $\hat{\lambda}_r$ the vertical axis. For large r these curves are flat: $\hat{\lambda}_r$ changes by less than 0.1 if $r > 62$ [33 if $ch^{\alpha} = 2$], less than 0.01 if $r > 105$ [97].

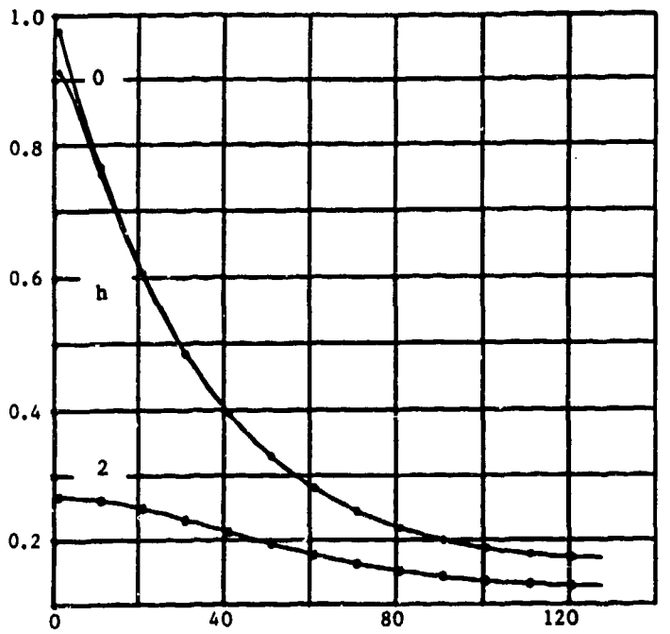

Figure 8. $\hat{\lambda}_r$ for ch^α = 0, h, 2.

If $\beta > 2$, the dominant term of the cluster radius $\delta(\beta,k)$ is a_k, for the term $d_k := b_\infty - b_{k+1}$ converges to 0 rapidly; this is shown in Table 1 below. When $\beta = 2$, $d_k = a_{k+1}$. $\delta(\beta,k)$ decreases as β or k increase.

k	a_k	d_k	$\delta(\beta,k)$	
4	.333-0	.226-0	.560-0	$\beta = 4 - 2\cos \pi h$
8	.142-0	.102-0	.244-0	b_∞ = .9759419-0
16	.652-1	.413-1	.106-0	
24	.413-1	.220-1	.632-1	
32	.294-1	.130-1	.424-1	
4	.330-0	.172-0	.502-0	$\beta = 2 + h$
8	.134-0	.571-1	.191-0	b_∞ = .9157456-0
16	.507-1	.112-1	.619-1	h = 1/129
24	.237-1	.262-2	.263-1	
32	.116-1	.633-3	.122-1	
4	.667-1	.920-4	.668-1	$\beta = 4$
8	.344-3	.245-8	.344-3	b_∞ = .2679492-0
16	.913-8	.173-17	.913-8	
24	.243-12	.122-26	.243-12	
32	.644-17	.0	.644-17	

Table 1. Cluster radii $\delta(\beta,k)$ for different k and β.

The jth factor $|\lambda^2-\hat{\lambda}_j^2|/|1-\hat{\lambda}_j^2|$ of $Q(\lambda,r)$ defined by (3.10) is no greater than 1 whenever $2\hat{\lambda}_j^2 \le 1+\lambda^2$. It is clear from (4.1, that $2\hat{\lambda}_j^2 \le 1$ whenever $\beta(j) \ge 3/\sqrt{2} \approx 2.12132$. Table 2 gives very pessimistic bounds on Q in terms of $\hat{Q}(r) := \Pi\{1/(1-\hat{\lambda}_j^2) : 2\hat{\lambda}_j^2 > 1, j \ne r\}$. Q is much smaller than $\hat{Q}$ because of the factors $|\lambda^2-\hat{\lambda}_j^2|$.

ch^α	$\hat{Q}(r)$
0	.3287627+9
h	.5976592+7
2	1

Table 2. Bounds $\hat{Q}(r)$ on the product $Q(\lambda,r)$.

References

[1] R. J. Arms, L. D. Gates, and B. Zondek, A method of block iteration, J. Soc. Ind. Appl. Math., 4 (1956), pp. 220-229.

[2] P. Concus, G. H. Golub, and D. P. O'Leary, A generalized conjugate gradient method for the numerical solution of elliptic partial differential equations, in Sparse Matrix Computations, J. R. Bunch and D. J. Rose, eds., Academic Press, New York, 1976, pp. 309-332

[3] J. W. Fischbach, Some applications of gradient methods, in Proc. Sympos. Appl. Math., J. H. Curtiss, ed., vol. 6, Numerical Analysis, McGraw-Hill, New York, 1956, pp. 59-72.

[4] A. Greenbaum, Comparison of splittings used with the conjugate gradient algorithm, Numerische Math., 33 (1979), pp. 181-193.

[5] M. R. Hestenes, The conjugate gradient method for solving linear systems, in Proc. Sympos. Appl. Math., J. H. Curtiss, ed., vol. 6, Numerical Analysis, McGraw-Hill, New York, 1956, pp. 83-102.

[6] M. R. Hestenes and E. Stiefel, Methods of conjugate gradients for solving linear systems, J. Research NBS, 49 (1952), pp. 409-436.

[7] E. Isaacson and H. B. Keller, Analysis of Numerical Methods, Wiley, New York, 1966.

[8] T. A. Manteuffel, An incomplete factorization technique for positive definite linear systems, Math. Comp., 34 (1980), pp. 473-497.

[9] S. V. Parter, Multi-line iterative methods for elliptic difference equations and fundamental frequencies, Numerische Math., 3 (1961), pp. 305-319.

[10] S. V. Parter and M. Steuerwalt, On k-line and k×k block iterative schemes for a problem arising in three-dimensional elliptic difference equations, SIAM J. Numer. Anal., 17 (1980), pp. 823-839.

[11] _____, Block iterative methods for elliptic and parabolic difference equations, in preparation.

[12] R. S. Varga, Matrix Iterative Analysis, Prentice-Hall, Englewood Cliffs, NJ, 1962.

[13] D. M. Young, Iterative Solution of Large Linear Systems, Academic Press, New York, 1971.